Lecture 13
Derivation of the S$_n$ Equations Via Collocation

1 Isotropic Scattering Case

The standard S_n equations in 1–D slab geometry with isotropic scattering can easily be derived using a collocation technique . We begin the derivation by choosing a set of N points on $[-1,+1]$ that are symmetrically arranged about $\mu = 0$, $\{\mu_m\}_{m=1}^{N}$. Next we obtain a trial space representation for the angular flux by interpolating these values. The interpolation scheme must act as a linear operator on the discrete angular flux vectors. That is to say that

$$H(a\overrightarrow{\psi^{(1)}} + b\overrightarrow{\psi^{(2)}}) = aH\overrightarrow{\psi^{(1)}} + bH\overrightarrow{\psi^{(2)}}\,, \tag{1}$$

where H is the interpolation operator that maps a vector of discrete angular flux values to a function on $[-1,+1]$, a and b are scalars, and $\overrightarrow{\psi^{(1)}}$ and $\overrightarrow{\psi^{(2)}}$ are any two discrete angular flux vectors:

$$\begin{aligned}
\overrightarrow{\psi^{(1)}} &= (\psi_1^{(1)}, \psi_2^{(1)}, \psi_3^{(1)}, \cdots, \psi_N^{(1)})\,, \\
\overrightarrow{\psi^{(2)}} &= (\psi_1^{(2)}, \psi_2^{(2)}, \psi_3^{(2)} \cdots, \psi_N^{(2)})\,.
\end{aligned} \tag{2}$$

In addition, the scheme must map the constant vector, $(1, 1, \cdots, 1)$, to the constant function, $\psi(\mu) = 1$. The trial space angular flux can be expressed as follows:

$$\psi(\mu) = \sum_{m=1}^{N} \psi_m B_m(\mu)\,, \tag{3}$$

where

$$\begin{aligned} B_1(\mu) &= H(1, 0, 0, \cdots, 0)\,, \\ B_2(\mu) &= H(0, 1, 0, \cdots, 0)\,, \\ B_N(\mu) &= H(0, 0, 0, \cdots, 1)\,. \end{aligned} \tag{4}$$

It follows from Eq. (4) that

$$B_m(\mu_j) = \delta_{m,j}\,, \quad m = 1, N\,, \tag{5}$$

and further that

$$\psi_m = \psi(\mu_m)\,, \quad m = 1, N. \tag{6}$$

There is a quadrature set that exactly integrates all elements of the trial space. The quadrature points correspond to the interpolation points that we have defined, and the weights are obtained simply by integrating Eq. (3):

$$2\pi \int_{-1}^{+1} \psi(\mu)\, d\mu = \sum_{m=1}^{N} \psi_m w_m\,, \tag{7}$$

where

$$w_m = 2\pi \int_{-1}^{+1} B_m(\mu)\, d\mu\,. \tag{8}$$

Because the interpolation is required to map the constant vector to the constant function, it follows that

$$\sum_{m=1}^{N} B_m(\mu) = 1.0 \quad . \tag{9}$$

Integrating (8), we find that the weights must sum to 4π:

$$\sum_{m=1}^{N} w_m = 2\pi \int_{-1}^{+1} d\mu = 4\pi \, . \tag{10}$$

To derive the S_n equations with angular (but not spatial) discretization, we first consider the transport equation with isotropic scattering and an isotropic distributed source:

$$\mu \frac{\partial \psi}{\partial x} + \sigma_t \psi = \frac{\sigma_s}{4\pi} \phi + \frac{q_0}{4\pi} \, . \tag{11}$$

Next we substitute from (3) into (10) and collocate at the interpolation (quadrature) points:

$$\mu \sum_{m=1}^{N} \frac{\partial \psi_m}{\partial x} B_m(\mu_k) + \sigma_t \sum_{m=1}^{N} \psi_m B_m(\mu_k) =$$
$$\frac{\sigma_s}{4\pi} \sum_{m=1}^{N} \psi_m w_m + \frac{q_0}{4\pi} \, , \quad k = 1, N. \tag{12}$$

Using Eq. (5), we simplify Eq. (12) as follows:

$$\mu_k \frac{\partial \psi_k}{\partial x} + \sigma_t \psi_k = \frac{\sigma_s}{4\pi} \phi + \frac{q_0}{4\pi} \, , \quad k = 1, N, \tag{13}$$

where

$$\phi = \sum_{m=1}^{N} \psi_m w_m \, . \tag{14}$$

Equation (14) is identical to the S_n equations (without spatial discretization) constructed from the quadrature set corresponding to our interpolatory trial space representation.

2 Anisotropic Scattering Case

With anisotropic scattering, the collocation process that we have defined does not necessarily yield the standard S_n equations. To demonstrate this, we first consider the transport equation with anisotropic scattering and an anisotropic distributed source:

$$\mu \frac{\partial \psi}{\partial x} + \sigma_t \psi = 2\pi \int_{-1}^{+1} \sigma_s(\mu' \to \mu) \psi(\mu') d\mu' + q \,. \tag{15}$$

Substituting from Eq. (3) into Eq. (15), and collocating at the quadrature points, we get an anisotropic distributed source:

$$\mu \frac{\partial \psi_k}{\partial x} + \sigma_t \psi_k = \sum_{m=1}^{N} S_{k,m} + q_k \,, \tag{16}$$

where

$$S_{k,m} = 2\pi \int_{-1}^{+1} \sigma_s(\mu' \to \mu_k) B_m(\mu') d\mu' \,. \tag{17}$$

The right side of Eq. (16) differs from the standard S_N equations. The main problem with this expression is that it is generally not conservative. Conservation requires that quadrature integration of Eq. (16) over all directions yield the balance equation:

$$\frac{\partial J}{\partial x} + \sigma_a \phi = Q_0 \,, \tag{18}$$

where

$$Q_0 = \sum_{m=1}^{N} q_k w_k \,. \tag{19}$$

This in turn requires that

$$\sum_{k=1}^{N} S_{k,m}\psi_m\, w_k = \sigma_s \phi\,, \quad m = 1, N. \tag{20}$$

If we assume that ψ is non-zero only in one direction, we find that Eq. (20) is equivalent to requiring that

$$\sum_{k=1}^{N} S_{k,m} w_k = w_m\,, \quad m = 1, N. \tag{21}$$

With an arbitrary scattering kernel, there is no reason to expect Eq. (21) to be satisfied.

To derive the S_N expressions for the scattering and inhomogeneous sources, we first follow Appendix C, and expand the scattering source and inhomogeneous sources in terms of finite-order Legendre expansions:

$$\mu\frac{\partial \psi}{\partial x} + \sigma_t \psi = \sum_{n=0}^{L} \frac{2n+1}{4\pi} \left(\sigma_n \phi_n + q_n\right) P_n(\mu)\,, \tag{22}$$

where $P_n(\mu)$ is the Legendre polynomial of degree n, and

$$\sigma_n = 2\pi \int_{-1}^{+1} \sigma_s(\mu_0) P_n(\mu_0)\, d\mu_0\,, \tag{23}$$

$$\phi_n = 2\pi \int_{-1}^{+1} \psi(\mu_0) P_n(\mu_0)\, d\mu_0\,, \tag{24}$$

$$q_n = 2\pi \int_{-1}^{+1} q(\mu_0) P_n(\mu_0)\, d\mu_0\,. \tag{25}$$

Using Eq. (3), we can re-express Eq. (24) in a more explicit manner:

$$\phi_n = \sum_{m=1}^{N} \psi_m w_m^{(n)}\,, \tag{26}$$

where

$$w_m^{(n)} = 2\pi \int_{-1}^{+1} B_m(\mu_0) P_n(\mu_0)\, d\mu_0 \, . \tag{27}$$

If we apply our collocation method to Eq. (22), we get

$$\mu \frac{\partial \psi_k}{\partial x} + \sigma_t \psi_k = \sum_{n=0}^{L} \frac{2n+1}{4\pi} \left(\sigma_n \phi_n + q_n\right) P_n(\mu_k) \, , \quad k = 1, N. \tag{28}$$

The scattering and inhomogeneous source terms in Eq. (28) are still not those used in the S_N method, but only because the angular flux moments are computed using the special quadrature weights defined by Eq. (27). Equation (28) represents the standard S_N equations when the angular flux moments are computed using the standard quadrature weights defined by Eq. (8):

$$\phi_n = \sum_{m=1}^{N} \psi_m P_n(\mu_m) w_m \, . \tag{29}$$

It is not difficult to see that Eq. (28) will be conservative whenever the quadrature weights exactly integrate the Legendre polynomials of degree K where $0 \leq K \leq L$. In particular, if we integrate the right side of Eq. (28) and assume that the quadrature set is exact for all polynomials appearing in the sum, we obtain the desired result

$$\begin{aligned} \sum_{k=1}^{N} \sum_{n=0}^{L} \frac{2n+1}{4\pi} \left(\sigma_n \phi_n + q_n\right) P_n(\mu_k)\, w_k &= \sum_{n=0}^{L} \frac{2n+1}{4\pi} \left(\sigma_n \phi_n + q_n\right) \sum_{k=1}^{N} P_n(\mu_k)\, w_k \\ &= \sigma_0 \phi_0 + q_0 = \sigma_s \phi + q_0 \, , \end{aligned} \tag{30}$$

which follows directly from the orthogonality of the Legendre polynomials. Thus we see that the standard S_n method requires the use of Legendre expansions when the scattering or inhomogenoeus sources are anisotropic. Furthermore, the accuracy of the quadrature set limits the order of the Legendre expansion that can be used.

In accordance with the derivation of the S_n equations given previously, all standard 1-D S_n quadrature sets are required to have quadrature points symmetric about $\mu = 0$. This ensures that the quadrature set will exactly integrate all Legendre polynomials of odd degree, and it preserves the symmetry of the 1-D slab-geometry transport equation. All standard 1-D S_n quadrature sets are also required to integrate μ^2. This is necessary to preserve the diffusion limit. For instance, if we assume P_1 scattering in Eq. (30), and a linear dependence for the angular flux, i.e.,

$$\psi_m = \frac{1}{4\pi}\phi + \frac{3}{4\pi}J\mu_m \,, \tag{31}$$

then substitute from Eq. (31) into Eq. (30), and successively take the zero'th and first angular moments of that equation using the quadrature formula, we get

$$\frac{3}{4\pi}\langle\mu^2\rangle\frac{\partial J}{\partial x} + \sigma_a\phi = Q_0 \,, \tag{32}$$

and

$$\frac{1}{4\pi}\langle\mu^2\rangle\frac{\partial \phi}{\partial x} + (\sigma_t - \sigma_1)J = 0 \,, \tag{33}$$

respectively, where we have assumed exact integration of all polynomials of odd degree, and

$$\langle\mu^2\rangle = \sum_{m=1}^{N} \mu_m^2 w_m \,. \tag{34}$$

Using Eq. (33) to eliminate the current from Eq. (32), we obtain a diffusion equation:

$$-\frac{\partial}{\partial x} D \frac{\partial \phi}{\partial x} + \sigma_a \phi = Q_0 \,, \tag{35}$$

where

$$D = \frac{3}{16\pi^2} \langle \mu^2 \rangle^2 \frac{1}{\sigma_0 - \sigma_1} \,. \tag{36}$$

Note from Eq. (36) that the correct diffusion coefficient will be obtain only if the quadrature set is exact for μ^2, i.e., if $\langle \mu^2 \rangle = 4\pi/3$.